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MINIMIZING CONVEX FUNCTIONS OVER A SIMPLEX

by

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SUMMARY

We present an iteration procedure to locate the minimum of a continuously differentiable strictly convex function over the unbounded simplex in Euclidean n -space, and we prove that the procedure converges to the unique minimum. This procedure is constructed to facilitate its adaptation to machine programming. Applications of this procedure to maximum likelihood estimation in certain non-parametric cases are mentioned.

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1. INTRODUCTION

Recently, there have occurred some applications of the problem of minimizing a convex function, say f , defined on Euclidean n -space R_n , over the unbounded simplex

$$S = \{(x_1, \dots, x_n) \in R_n : x_1 \leq x_2 \leq \dots \leq x_n\}.$$

Special cases of this problem arise in the maximum likelihood estimation of parameters subject to known constraints. These problems have been treated by Brunk et al in a series of papers [1], [2], [3]. They also arise in the maximum likelihood estimation in certain non-parametric situations as treated by Marshall and Proschan [5].

The method used in the cases cited requires that the function f be of the form

$$(1.1) \quad f(x_1, \dots, x_n) = \sum_1^n f_i(x_i)$$

where each f_i is convex over R_1 .

Let $u(j-r, j+s)$ be the value of x which minimizes $\sum_{i=j-r+1}^{j+p-1} f_i(x)$. Then the minimizing point of f over the

simplex S , call it (a_1, \dots, a_n) , is known to be given by

$$a_j = \max_{r \geq 1} \min_{s \geq 1} u(j-r, j+s).$$

This straightforward method works for non-parametric estimates in the case of densities with increasing failure rates.

The general problem of minimizing a function over compact subsets of R_n in the case the function is strictly convex in each coordinate and continuously differentiable and assumes the minimum in the interior has been treated by Warga [6]. He proposes the use of an iteration procedure of minimizing successively one coordinate after another beginning at any point.

If f is convex and continuously differentiable in R_n and is to be minimized over the bounded simplex

$$S_M = \{(x_1, \dots, x_n) \in R_n : -M \leq x_1 \leq \dots \leq x_n \leq M\}$$

for some $M > 0$, then one may utilize the Warga iteration procedure to find the minimum of f over the n -fold Cartesian product of the interval $[-M, M]$. Let it be (a_1^*, \dots, a_n^*) . Then knowing the result (proved in [3]) that if $a_j^* > a_{j+1}^*$, then the point (a_1, \dots, a_n) which minimizes f over S_n must have $a_j = a_{j+1}$. We can, in at most n applications of the Warga procedure, obtain the minimum over S_M .

The problem which arises in the determination of the nonparametric maximum likelihood estimate in the case the density has

a convex failure rate is that of minimizing a convex function (which does not have property (1.1)) over the unbounded simplex. The belief which prompted this effort was that something could be found which was alternate to the method above for some M sufficiently large.

2. THE ITERATION OPERATOR

Let f be a function which is to be minimized over the convex set S . We assume that f satisfies the following:

1° For any $\alpha, \beta \in S$ and $t \in (0,1)$

$$f(t\alpha + (1-t)\beta) < tf(\alpha) + (1-t)f(\beta),$$

and letting δ_i be the vector which is zero in every coordinate except the i^{th} which is unity, we have

$$D_j f(\alpha) = \lim_{t \rightarrow 0} \frac{f(\alpha + t\delta_j) - f(\alpha)}{t},$$

the partial derivative with respect to the j^{th} coordinate, exists and is continuous for $j = 1, \dots, n$.

2° If $\{\alpha^i\}$ is a sequence of points in S such that at least one coordinate, say the j^{th} , has the property that

$$\limsup_{i \rightarrow \infty} |\alpha_j^i| = \infty \quad \text{then} \quad \limsup_{i \rightarrow \infty} f(\alpha^i) = \infty.$$

Now from 1° it follows that f is a strictly convex continuously differentiable function and from 2° that a minimizing value of f over

S exists which by the strict convexity must be unique.

For any vector $\alpha \in S$ and any two integers j, k such that $j \geq 1$, $k \leq n$ and $k \geq j$ we make the notational convention for x a real number

$$(2.1) \quad (x; v, k, \alpha) = \alpha + x(\delta_j + \dots + \delta_k)$$

where $\delta_i = (\delta_{1i}, \delta_{2i}, \dots, \delta_{ni})$ with δ_{ji} the Kronecker delta.

Now if we use Δ as the difference operator $\Delta\alpha_j = \alpha_j - \alpha_{j-1}$, then $-\Delta\alpha_j \leq x \leq \Delta\alpha_{k+1}$ implies that $(x; j, k, \alpha) \in S$. Let the value of $x \in [-\Delta\alpha_j, \Delta\alpha_{k+1}]$ which minimizes $f(x; j, k, \alpha)$ be denoted by $p(j, k, \alpha)$.

LEMMA 1: For given integers such that $j \geq 1$, $k \leq n$, $k \geq j$ we have

$p(j, k, \alpha)$ is a continuous function of α on S .

PROOF: Let j, k as required and $\alpha \in S$ be fixed arbitrarily. To show continuity, let $\{\alpha^n\}$ be a sequence of points in S such that $\alpha^n \rightarrow \alpha \in S$. If $p_{n_1} = p(j, k, \alpha^n)$ does not converge to $p(j, k, \alpha)$, then by compactness there is a subsequence such that

$$p_{n_1} \rightarrow p_0 \neq p(j, k, \alpha)$$

CASE I $-\Delta\alpha_j < \Delta\alpha_{k+1}$. Take $x \in (-\Delta\alpha_j, \Delta\alpha_{k+1})$. Then for that x there is an N sufficiently large that

$$x \in \bigcap_{i > N} \left[-\Delta\alpha_j^{n_i}, \Delta\alpha_{k+1}^{n_i} \right]$$

and then for $i > N$, we have

$$f(p_{n_i}; j, k, \alpha^{n_i}) \leq f(x; j, k, \alpha^{n_i}).$$

Now letting $i \rightarrow \infty$, we have by continuity of f that

$$f(p_0; j, k, \alpha) \leq f(x; j, k, \alpha).$$

This inequality holds for arbitrary $x \in (-\Delta\alpha_j, \Delta\alpha_{k+1})$ and by continuity of f must hold for all x in the closed interval.

Hence, by strict convexity, it must follow that p_0 is the minimizing value and by definition $p_0 = p(j, k, \alpha)$ which is a contradiction.

CASE II $-\Delta\alpha_j = \Delta\alpha_{k+1}$. Since $\Delta\alpha_1 \geq 0$, we must have $\Delta\alpha_j = \Delta\alpha_{k+1} = 0$ and since $\alpha^n \rightarrow \alpha$ it must follow that $|\Delta\alpha_j^n| + |\Delta\alpha_{k+1}^n| \rightarrow 0$ as $n \rightarrow \infty$. But $-\Delta\alpha_j^n \leq p_n \leq \Delta\alpha_{k+1}^n$ and hence $p_n \rightarrow 0 = p(j, k, \alpha)$. This completes the proof.

We now define the transformations

$$(2.2) \quad A_{jk}(\alpha) = \alpha + p(j, k, \alpha)(\delta_j + \dots + \delta_k) \quad \text{for } 1 \leq j \leq k \leq n.$$

Following immediately from Lemma 1 we make the obvious

REMARK: For each j, k as prescribed, the transformation A_{jk} is a continuous map from S into S .

In turn, we set

$$\begin{aligned} A_1 &= A_{nn} \cdots A_{jj} \cdots A_{22}A_{11} \\ . &. \\ (2.3) \quad A_r &= A_{n+1-r,n} \cdots A_{2,r+1}A_{1r} \\ . &. \\ A_n &= A_{1n} \end{aligned}$$

where juxtaposition indicates composition of the transformations.

Finally, we set

$$(2.4) \quad B = A_n \cdots A_2 A_1.$$

Since the composition of continuous functions is continuous, we have

THEOREM 1: The transformation B is a continuous map of S into itself.

We now prove

LEMMA 2: If $A_{jk}(\alpha) \neq \alpha$, then $f(A_{jk}(\alpha)) < f(\alpha)$.

PROOF: By definition

$$f(A_{jk}(\alpha)) \leq f(\alpha + x\delta_j + \dots + x\delta_k) \quad \text{for all } x \in [-\Delta\alpha_j, \Delta\alpha_{k+1}]$$

and by strict convexity we obtain equality iff $x = p(j,k,\alpha)$.

Since always $0 \in [-\Delta_{j,k}, \Delta_{j,k+1}]$ for $\alpha \in S$ we have $f(A_{j,k}(\alpha)) \leq f(\alpha)$ with equality iff $p(j,k,\alpha) = 0$. Clearly then $p(j,k,\alpha) \neq 0$

implies $f(A_{jk}(\alpha)) < f(\alpha)$ and by equation 2.3 it follows that $A_{jk}(\alpha) \neq \alpha$ iff $p(j,k,\alpha) \neq 0$. This completes the proof.

3. PROOF OF CONVERGENCE

Definition: A point $\alpha \in S$ is a *fixed point* of B iff

$$B(\alpha) = \alpha.$$

One checks easily that the property of the A_{jk} 's expressed in Lemma 2 is preserved under composition. Thus, we have

THEOREM 2: B is a transformation defined from S into S such that if α is not fixed, then $f(B\alpha) < f(\alpha)$.

There follows immediately

THEOREM 3: If μ is the unique minimum of f over S , then μ is a fixed point of B .

PROOF: Otherwise, by Theorem 2 $B(\mu) \neq \mu$ which would contradict the fact that μ was the minimum.

We now derive some properties of this minimum which shall be needed subsequently. We define

$$(3.1) \quad \partial f(\alpha; \beta - \alpha) = \lim_{t \rightarrow 0} \frac{1}{t} [f(\alpha + t\beta - t\alpha) - f(\alpha)]$$

and as we know we have

$$(3.2) \quad = \sum_1^n (\beta_i - \alpha_i) D_i f(\alpha).$$

In the above, we have followed the notation of [4].

LEMMA 3: Suppose the minimum μ of f is such that

$$\mu_{j-1} < \mu_j = \dots = \mu_k < \mu_{k+1} \quad \text{for } j < k$$

then it follows that for $j \leq r \leq k$

$$(3.4.1) \quad \partial f(\mu; \sum_r^k \delta_i) = \sum_r^k D_i f(\mu) \geq 0,$$

$$(3.4.2) \quad \partial f(\mu; \sum_j^r \delta_i) = \sum_j^r D_i f(\mu) \leq 0$$

and

$$(3.4.3) \quad \partial f(\mu; \sum_j^k \delta_i) = \sum_j^k D_i f(\mu) = 0$$

PROOF: If γ is any point in S , then

$$(3.5) \quad \partial f(\mu; \gamma - \mu) = \sum_1^n (\gamma_i - \mu_i) D_i f(\mu) \geq 0,$$

otherwise μ would not be the minimum since there would exist a

$t \geq 0$ such that

$$\frac{1}{t} [f(\mu + t(\gamma - \mu)) - f(\mu)] < 0$$

which would be a contradiction to μ being the minimum. Now take

$$\gamma_i = \begin{cases} \mu_j - x & i = j, \dots, r \\ \mu_i & i \text{ otherwise.} \end{cases}$$

For some $x > 0$ such that $\gamma \in S$ it follows

$$\sum_1^n (\gamma_1 - \mu_1) D_1 f(\mu) = -x \partial f(\mu: \sum_1^r \delta_1) \geq 0.$$

This proves (3.4.2). The other case is done similarly. The proof of (3.4.3) follows immediately as a corollary since we must have the l.h.s. both ≥ 0 and ≤ 0 .

We can now state the crucial

THEOREM 4: If α is not the minimum of f over S , then α is not a fixed point of B .

By (3.3) we have

$$(3.6) \quad \partial f(\alpha: \mu - \alpha) = \sum_{j=1}^r (\mu_j - \alpha_j) D_j f(\alpha) < 0.$$

If we consider the intervals of indices across which α_i is constant, say,

$$1 = \ell_0 \leq i < \ell_1, \ell_1 \leq i < \ell_2, \dots, \ell_N \leq i < \ell_{N+1} = n+1$$

we may rewrite (3.6) as

$$(3.7) \quad \partial f(\alpha: \mu - \alpha) = \sum_{i=1}^N \sum_{j=\ell_i}^{\ell_{i+1}-1} (\mu_j - \alpha_{\ell_i}) D_j f(\alpha) < 0.$$

Since α is a fixed point of B we must have over each interval in which α_i is constant,

$$(3.7.1) \quad \partial f(\alpha: \delta_{\ell_j} + \dots + \delta_{-1+\ell_{j+1}}) = 0 \quad j = 0, \dots, m$$

otherwise α would not be a fixed point of $A_{\ell_j, -1+\ell_{j+1}}$.

Moreover, for every $j = 0, \dots, m$, we must have for each

$$\ell_j \leq k < \ell_{j+1}$$

$$(3.7.2) \quad \partial f(\alpha: \delta_{\ell_j} + \dots + \delta_k) \leq 0$$

$$(3.7.3) \quad \partial f(\alpha: \delta_k + \dots + \delta_{-1+\ell_{j+1}}) \geq 0$$

otherwise, α would not be fixed for the appropriate $A_{j,k}$'s.

Since the sum in (3.7) is negative, it follows that at least one of the summands must be negative. Suppose without loss of generality that it is the first. If we also consider the subintervals of $\ell_1 \leq j < \ell_2$ across which μ_j is constant, say for some $N \geq 1$,

$$\ell_1 = k_1 \leq j < k_2, \quad k_2 \leq j < k_3, \dots, k_m \leq j < k_{m+1} = \ell_2.$$

We have from (3.7) by using (3.2) that

$$(3.7.4) \quad \sum_{i=0}^m (\mu_{k_i} - \alpha_{\ell_1}) \partial f(\alpha: \delta_{k_i} + \dots + \delta_{-1+k_{i+1}}) < 0.$$

If μ_j is constant across $\ell_1 \leq j \leq \ell_2$ (i.e. $m = 1$ in (3.7.4)), then we have a contradiction with (3.7.1). Thus, we

assume $m > 1$. Because μ_{k_1} is an increasing function of i it must cross α_{ℓ_1} at most once. Thus, we can write (3.7.4) as

$$(3.7.5) \quad 0 > \left(\sum_{i=1}^s + \sum_{i=s+1}^m \right) (\mu_{k_1} - \alpha_{\ell_1}) \partial f(\alpha: \delta_{k_1} + \dots + \delta_{-1+k_{i+1}}).$$

On the right-hand side of (3.7.5) we label the first sum I and the second II where

$$(3.7.6) \quad \begin{aligned} \mu_{k_i} &\leq \alpha_{\ell_1} & \text{for } i = 1, \dots, s \\ \mu_{k_i} &> \alpha_{\ell_1} & \text{for } i = s+1, \dots, m \end{aligned}$$

and perhaps one of the summations is vacuous.

Consider the first term of I keeping (3.7.2) and (3.7.6) in mind. Now

$$(\mu_{k_1} - \alpha_{\ell_1}) \partial f(\alpha: \delta_{k_1} + \dots + \delta_{-1+k_2}) \geq 0.$$

Since μ_{k_i} is an increasing function of i , we have also

$$0 \leq (\mu_{k_2} - \alpha_{\ell_1}) \partial f(\alpha: \delta_{k_1} + \dots + \delta_{-1+k_2}) \leq (\mu_{k_1} - \alpha_{\ell_1}) \partial f(\alpha: \delta_{k_1} + \dots + \delta_{-1+k_2}).$$

By combining the terms $i = 1, 2$, we have

$$\begin{aligned} I \geq \sum_{i=3}^s (\mu_{k_2} - \alpha_{\ell_1}) \partial f(\alpha: \delta_{k_1} + \dots + \delta_{-1+k_{i+1}}) \\ + (\mu_{k_2} - \alpha_{\ell_1}) \partial f(\alpha: \delta_{k_1} + \dots + \delta_{-1+k_3}). \end{aligned}$$

Repeating the argument s times we see that eventually we show

$$I \geq (\mu_{k_s} - \alpha_{\ell_1}) \partial f(\alpha; \delta_{k_1} + \dots + \delta_{-1+k_{s+1}}) \geq 0.$$

A similar argument holds for showing $II \geq 0$ and thus we have a contradiction to (3.7.5).

We now have

THEOREM 5: For any $\alpha \in S$ the sequence $\{B^n(\alpha)\}$ converges to a fixed point of f .

PROOF: Let $\alpha^n = B^n(\alpha)$ for $n = 1, 2, \dots$ then the sequence $\{\alpha^n\}$ has a convergent subsequence since it is from the set $\{\beta \in S : f(\beta) \leq f(\alpha)\}$ which is closed and bounded by virtue of 2° and being a subset of Euclidean n -space is compact. Set $a_n = f(\alpha^n)$. The sequence $\{a_n\}$ is a decreasing sequence of real numbers bounded below and therefore converges to a_0 , say. Clearly all limit points of $\{\alpha^n\}$ have the same f value, namely a_0 .

Let $\alpha^{n_k} \rightarrow \gamma$, say, then

$$b_0 = f(\gamma) \leq f(B(\alpha^{n_k})) \leq f(\alpha^{n_k})$$

and letting $k \rightarrow \infty$ we have

$$\lim_{k \rightarrow \infty} fB(\alpha^{n_k}) = f(\gamma).$$

But by Theorem 1, B is continuous and by assumption f is also thus we have

$$\lim_{k \rightarrow \infty} fB(\alpha^{n_k}) = fB(\gamma)$$

and $fB(\gamma) = f(\gamma)$ and γ is a fixed point which is the unique minimum.

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